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Atomistic modeling of diffusion coefficient in fusion reactor first wall material tungsten

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HIGHLIGHTS

- Self-diffusion coefficients of fusion reactor material tungsten have been analyzed.
- Dipole interaction model is introduced to analyze diffusion in the magnetic field.
- Tungsten diffusion activation energy increases in the strong uniform magnetic field.
- The strong uniform magnetic field limits the diffusion coefficient of tungsten.

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ABSTRACT

Tungsten is remarkable for its robustness, especially it has the highest melting point of all the non−alloyed metals. Metallic material tungsten and tungsten alloys have been widely used in aerospace, weapon, nuclear industries and fusion reactor. Tungsten is expected to be the fusion reactor first wall material for this reason. In this paper, self-diffusion coefficients of metallic material tungsten have been investigated via molecular dynamics simulation method using the modified embedded atom potential model. Diffusion activation energy of tungsten can be gotten according to Arrhenius relation between the self-diffusion coefficients simulation results and temperatures. The dipole interaction model is introduced to analyze metallic material tungsten self-diffusion process in a uniform magnetic field. The strong magnetic field increases diffusion activation energy by 34.52% and limits self-diffusion coefficient by 1.15% in 2 T uniform magnetic field.

1. Introduction

Because of the shortage of fossil energy and environmental pollution, fusion energy has been emphasized by scientists and international organizations to take the place of gradually scarce traditional energy. The plasma irradiation effects and fusion reactor first wall diffusion process would probably shorten the lifetime of first wall and change material properties, thus plasma facing materials is one of great scientific challenges for development and design of magnetic confinement fusion reactor. Tungsten is remarkable for its robustness, especially it has the highest melting point of all the non−alloyed metals. Tungsten is expected to be the fusion reactor first wall material for this reason. Tungsten has some good features [1], such as high melting point, high thermal conductivity, strong corrosion resistance and low thermal expansion coefficient. Therefore, tungsten is the most potential material for first wall and a tungsten−coating fusion device has been proposed in 2004 [2].

Diffusion processes exist in atomic energy technology, metallurgical engineering and other industrial processes. Diffusion coefficient is an important foundation data in the mass transfer process and industrial equipment design. So far, scientists have not found ideal theoretical model of liquid metal diffusion process, resulting in the difficulties to explain the diffusion process of liquid metal. Inert hard sphere model achieved successful explanation on some chemical and physical properties of materials. Molecular dynamics simulation method has a certain similarity with the inert hard sphere model in atom movement and collision processes. Molecular dynamics simulation method would be helpful to deeply understand the thermal properties and transport process mechanism based on the statistical thermodynamics physics. In the fusion reactor design, mass transfer property of tungsten coating and film is one of important and fundamental scientific data. Many studies [3–5] have focused on the basic thermal and transport properties

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and described thermal expansion coefficient, melting processes, thermal conductivity and diffusion coefficient for tungsten and other materials. There are still some difficulties to simulate heat transport processes for metal by using classical MD method because of electronic contribution. Using molecular dynamics method, Chamati [6] researched iron self-diffusion using embedded-atom model (EAM) potential, and Wang [7,8] researched diffusion of liquid lithium and liquid lead which showed feasibility of molecular dynamics simulation method to study the material physics and chemistry properties. A correlation of the W-diffusion coefficient was developed by Mundy et al. [9] which gave the calculation of the self-diffusion coefficient of W self diffusion coefficient and measured self-diffusion in tungsten single crystals and obtained calculating formula for self-diffusion over the 1700–3400 K temperature range. No experimental results are reported in extreme high temperature environment because of no melt resistant container to place liquid tungsten. Bowden et al. [10] described briefly the results of some recent experiments on the diffusion of tungsten atoms over an atomically clean surface of tungsten and the method for the determination of the surface self-diffusion coefficient. Graham et al. [11] established quantitatively the tungsten surface diffusion parameters. Choi et al. [12] investigated tungsten self-diffusion on terraces by the field-emission fluctuation method. For fusion reactor, many researches were focused on the diffusion behavior of H within tungsten [13,14]. So far, metallic material tungsten and tungsten alloys have been widely used in aerospace, weapon, nuclear industries and fusion reactor where many extreme conditions have been demanded. Phase transformation processes of fusion reactor first wall material tungsten had been investigated via molecular dynamics simulation based on the modified embedded atom model as the basis for this study [15]. Accordingly, it is essential to provide detail diffusion coefficient database on the diffusion processes of tungsten in the high temperature and high magnetic field. In this paper, self-diffusion processes of tungsten single crystals over higher temperature range (3900 K-5700 K) are studied using molecular dynamics simulation method, and dipole interaction model is introduced to analyze the diffusion processes in a uniform magnetic field.

2. Molecular dynamic simulation

The embedded–atom method (EAM) based on density–functional theory was developed for some face-centered cubic (FCC) and body-centered cubic (BCC) metals, then Baskes et al. modified the EAM to include directional bonding that is necessary to explain the behavior of non–FCC materials, and extended it to a large number of elements [16]. In this paper, modified embedded–atom method (MEAM) potential [17] has been used here to describe the interactions between tungsten atoms, which have been applied into studying the crystalline structure and physical properties of metals. The potential energy equations of the system can be given as follows from equation (1) to equation (6).

$$U = \sum_i \left\{ \mathrm{F}_i(\overline{\rho}_i) + \frac{1}{2}\sum_{i\neq j}\phi_{ij}(r_{ij}) \right\} \tag{1}$$

where $\phi_{ij}(r_{ij})$ is the pair potential between atom i and atom j, $\mathrm{F}_i(\overline{\rho}_i)$ is the embedding energy function, and $\overline{\rho}_i$ is the environmental electron density at the position of atom i. $\mathrm{F}_i(\overline{\rho}_i)$ is expressed as

$$\mathrm{F}_i(\overline{\rho}_i) = A_i E_i^0 \overline{\rho}_i \ln\overline{\rho}_i \tag{2}$$

where A_i is adjustment factor, E_i^0 is the cohesive energy.

$\phi_{ij}(r_{ij})$ is expressed as:

$$\phi_{ij}(r_{ij}) = \overline{\phi}_{ij}(r_{ij}) S_{ij} \tag{3}$$

$$\overline{\phi}_{ij}(r_{ij}) = \frac{1}{Z_{ij0}}\left[2E_i^u(r_{ij}) - F_i\widehat{\rho}_i(r_{ij}) - F_j\widehat{\rho}_j(r_{ij})\right] \tag{4}$$

$$E_i^u\left(r_{ij}\right) = -E_{ij}^0\left(1 + a_{ij}^*(r_{ij})\right)e^{-a_{ij}^*(r_{ij})} \tag{5}$$

$$a_{ij}^* = \alpha_{ij}\left(\frac{r_{ij}}{r_{ij}^0} - 1\right) \tag{6}$$

where E_{ij}^0, r_{ij}^0, α_{ij}^0 are related parameters with atom i and j, Z_{ij0} is decided by atoms mutual structure in simulation system. $\widehat{\rho}_j(r_{ij})$ is the environmental electron density effect on the r_{ij}. S_{ij} is the scanning function decided by the cut-off radius.

The simulation system is designed for uniform melting simulation. We build a prefect bcc tungsten crystal box and the dimension of the simulation box is $10a \times 10a \times 10a$ in [1 0 0], [0 1 0] and [0 0 1] directions, respectively. Periodic boundary conditions are executed all these three directions. The symbol a, initial lattice constant, is 0.31652 nm at 0K. In the simulation, we have first carried out a constant temperature and pressure (NPT) simulation based on the simulation box for a prefect bcc tungsten crystal to obtain the thermal expansion coefficient at a given temperature range. Uniform melting point can also be estimated by a step-change of volume of tungsten crystal box. Then a canonical ensemble (NVT), using corresponding lattice constant, is applied to calculations of physical properties. In the simulation, the inputted heat is controlled by the constant temperature reservoir using NPT or NVT method in molecular dynamics simulation. Time step is 1 fs, and temperature increases 100 K every 10,000 steps. The system should be equilibrated at predetermined temperature for 5×10^5 time steps, which are sufficient and necessary to get reliable results.

3. Uniform melting and self-diffusion

In fact, the selection and design of materials that will withstand the extreme conditions of a fusion power plant. The fusion power plant is known as one of the greatest materials science challenges in history. The high particle flux, high thermal load and thermal mechanical stress combine to produce a uniquely hostile environment. Although tungsten has the second highest melting point of all the elements after graphite, using in fusion power plant, graphite have a major disadvantage–its high reactivity with hydrogen. Hydrogen would come into contact with surface carbon to form volatile hydrocarbons that are re-deposited in a different part of the vessel. It is a major problem for the tritium inventory because of both resource and safety issues. The fusion power plant uses tungsten as a favored plasma-facing because of its high melting temperature and thermal conductivity. In high temperature environment, tungsten may near melting point. So, we need further research tungsten uniform melting processes and self-diffusion in the high temperature and high uniform magnetic field.

NPT ensemble is employed to simulate crystal expansion processes. As shown in Fig. 1, the perfect lattice structure of simulation system is destroyed gradually with increasing temperature and then perfect crystals system become irregular liquid system. Melting process is a complex physical problem, it includes convection and conduction processes from the microscopic point of view. But in macro perspective, the movement of atom is the only and important description for the melting process.